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Published in:
12th Conference on Sustainable Development of Energy, Water and Environment Systems (SDEWES 2017), Oct 4-8, 2017, Dubrovnik, Croatia

Published: 04/10/2017

Document Version
Peer reviewed version

Link to publication on the UWS Academic Portal

Citation for published version (APA):
Alanazi, A., Tosin, I., Awotwe, T. W., Vichare, P., & Olabi, A-G. (2017). Performance evaluation of air breathing PEMFC under Saudi Arabia's ambient conditions using three-dimensional FEM model. In *12th Conference on Sustainable Development of Energy, Water and Environment Systems (SDEWES 2017), Oct 4-8, 2017, Dubrovnik, Croatia*

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Performance evaluation of air breathing PEMFC under Saudi Arabia's ambient conditions using three-dimensional FEM model

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ABSTRACT

In 2016, Saudi Arabia has announced a new vision for year 2030, and set an initial target of 9.5GW to be generated from renewable energy sources [1]. Air-breathing proton exchange membrane fuel cell (PEMFC) stack is seen as a promising candidate as an alternative source of energy to conventional combustion engines in stationary and automotive applications. This type of PEMFC uses ambient air as the oxidant and hydrogen as the fuel generating electricity. The performance of air-breathing PEMFC is highly affected by the operating ambient conditions, such as temperature and humidity. In this paper, the performance of an air breathing PEMFC is evaluated under Riyadh's city ambient conditions throughout the year, to help policy-makers in considering deploying this technology in the new public transportation project in the city, which is due to complete in 2019. Thermal and water management is obtained though validated 3-dimensional model. Furthermore, the effect of anode humidification on the dynamics of the PEMFC is analysed.

KEYWORDS

Hydrogen storage, renewable energy, PEMFC simulation, energy storage.

INTRODUCTION

Due to the increase of the population growth and infrastructure development projects which are supported by the abundant oil and natural gas resources, the Kingdom of Saudi Arabia (KSA) is considered to be among the countries with the highest energy use per capita in the world [2]. In additional to this, in the last 20 years KSA saw a dramatic increase in carbon emissions of over 70% change [3]. A major contribution to the KSA's emissions comes from the transportation sector that account for around 23% of the total energy consumption in the country, and this is expected to grow as the demand for personal vehicles continue to rise [4]. In an effort to diversify KSA's fossil fuel-based energy, in 2016 the Saudi government announced Vision 2030, which is an ambitious plan with a set of goals to be achieved by year 2030. Along the goals, is to generate 9.5GW from renewable and clean resources such as solar and nuclear power [1].

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PEM Fuel cells are seen as a promising clean source of energy for transportation applications, and they are devices that converts the chemical reaction of Hydrogen with Oxygen to produce electrical energy, water and heat. These devices are gaining significant interest mainly because they are pollution-free and two to three times more efficient than conventional combustion engines [5]. Extensive progress has been made in the last decade in the research and development of this technology (figure 1 shows a fuel cell stack). A number of leading automotive companies have successfully developed fuel cell versions of vehicles to their production line, such as Toyota Mirai and Honda Clarity [6,7]. Furthermore, several governments have funded fuel-cell-powered transportation projects in recent years. In China, the province of Qingdao deployed the first fuel cell tram in the country in 2016 [8]. Also the Chinese government have invested $72 million to fund a new plant that will manufacture fuel cell powered trams in 2016 [9]. Meanwhile, Germany have conducted successful trials on the world's first hydrogen-powered train, also known as Hydrail, and the first operational trains are expected to commence in 2018 [9]. Moreover, Europe's largest fleet of hydrogen fuel cell buses was deployed in Aberdeen, Scotland. This project was completed and the buses became fully operational in 2015. The project which was funded by public and private sectors costed £19m and compromised 10 hydrogen buses, 3 electrolysers to produce hydrogen on site, a refuelling station and a maintenance facility [10,11].

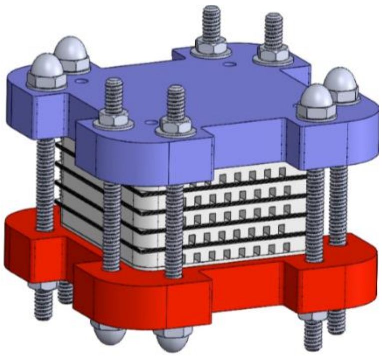


Figure 1: Air breathing fuel cell stack

Figure 2. Hydrogen buses in Aberdeen

Despite the outstanding achievements and the promising prospects for fuel-cell powered vehicles, there are a number of challenges that needs addressing before this technology can commercially be competing with existing combustion engines. These challenges include the hydrogen availability and infrastructure, fuel cell cost and durability, and technological advancement. From a technological aspect, the air-breathing concept of the fuel cell reduces the complexity of the overall system, as it eliminates the need for some of the balance-of-plant components for the cathode side such as humidifier, compressor, and cooling unit (figure 2). This utilises the ambient air as the oxidant, and directly feeds it to the cathode. Thus, this design has an encouraging potential to be used in fuel-cell powered vehicles, as it reduces the space

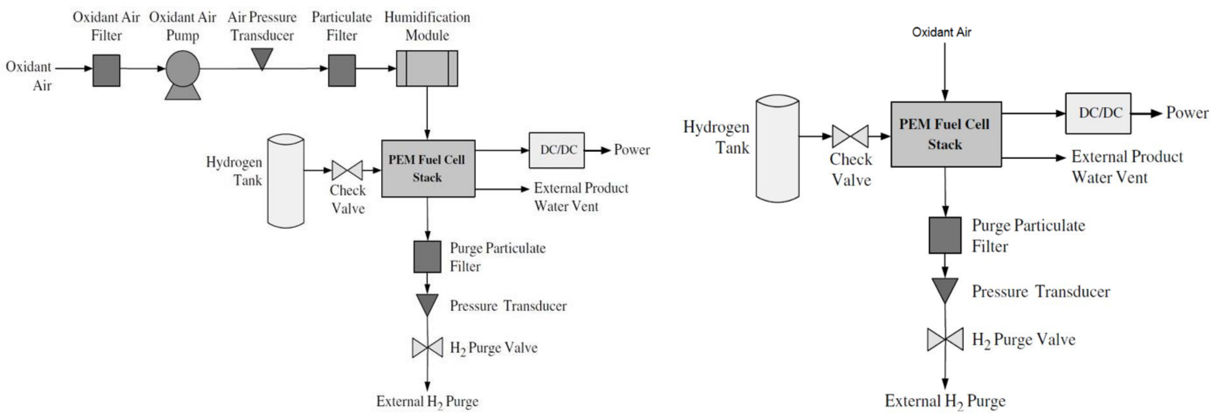


Figure 3. Fuel cell system 3.1) conventional process design 3.2) air-breathing process design [12]

and the weight of the system. However, the performance air-breathing PEMFC depends highly on the incoming air's ambient conditions, namely, humidity and temperature, and this cannot be maintained. Therefore, at the times of fluctuations of air conditions, the anode-side, is usually controlled to keep the performance at a steady level.

Riyadh's public transportation project

Due to the rapid increase of the population in the capital city of KSA, Riyadh, the High Commission of Arriyadh (HCA) announced the public transportation project in late 2011 with the main goal to reduce both traffic congestion and pollution in the city. According to studies conducted by the HCA the population in Riyadh is expected to rise from 6 million to 8 million with the next 10 years. The public transportation project costs $22.5 billion and the first phase is scheduled to become operational in 2019. This mega-project compromises a metro network with four main stations and six lines with a total length of 110 miles, and a bus network with 22 lines. Figure 4 shows the proposed metro lines in the city.

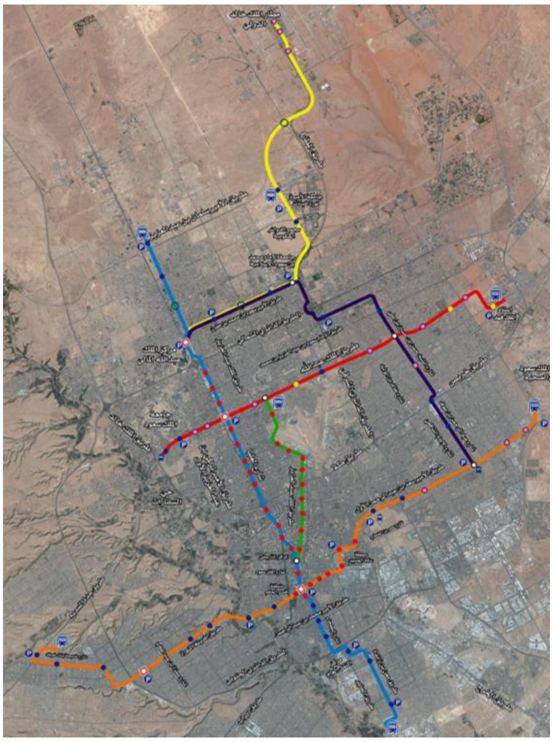


Figure 4. Map view of the proposed metro lines

The power source for the metro trains will be electricity and the power needed is estimated to be 468 MVA. Each metro line will be provided by electric power from two independent sources, i.e. there will be 12 power plants to feed this project. In addition, the buses will be running using diesel fuel with low sulphur content [13].

Hydrogen production in Saudi Arabia

Currently significant amount of Hydrogen is being produced in Saudi Arabia to support crude oil refineries as well as metal and petrochemical industries. The hydrogen is consumed on-site as a raw material for different compounds, such as ammonia. In 2014, Air Liquide started the production of a global-scale hydrogen plant in Yanbu, with a total capacity of 340,000 Nm^3/h [14]. However, the plant uses steam-reforming process and produce high emissions of carbon dioxide, i.e.5.5 kg for every kg of H_2 produced.

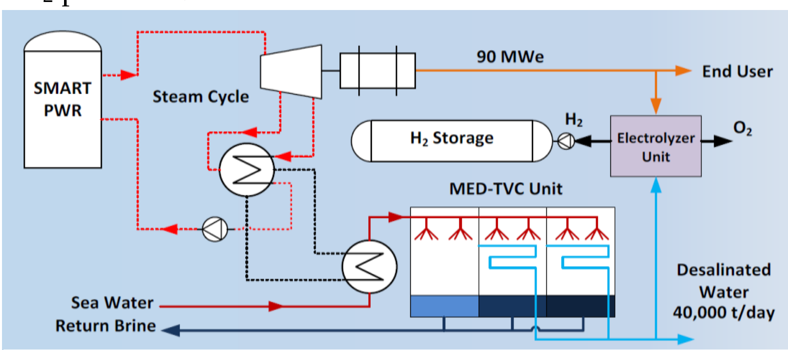


Figure 5. Proposed process design to produce Hydrogen from nuclear plant

To improve the hydrogen infrastructure in the country while maintaining the increased demand and achieving lower carbon emissions, carbon capture and storage equipment can be used in plant sites. Furthermore, Hydrogen can be produced without carbon footprint through electrolysis using a clean source of energy such as solar or nuclear. Abdullah [15] suggested a process design (figure 5) to produce hydrogen. This design integrates water desalination to the electrolyser system and uses electric power from the currently being built SMART nuclear reactor in KSA.

Relevant studies

D.T. Santa Rosa et. al. studied the effect of PEM fuel cell stack with an open cathode at high performance in ambient conditions such as flow rate, cell temperatures and hydrogen pressure. An external air fan was used at the cathode which will combine with oxidant supply and serve in cooling the stack. They discovered that the stack performed better when in operation with forced air convection than natural air convection. It was concluded that when the fuel stack is in operation under dead end hydrogen flow the cell performance is higher [16]. For anode humidification, Tabbi et.al. carried out an experiment of an open circuit voltage of anode humidification of the cell to observe the effect on the cell performance. It was noticed that has the pressure is being varied the polarization curve increases considerably to 4.5v in a fair amount. The cell was generating current of 6A and the polarization curve was observed to be constant at the beginning but there was deviation in the curves at a current higher densities. Also, it was noticed that when the fuel cells reaches the utmost current it can produce the voltage drops. They concluded that anode humidification is important in fuel cell performance [17]

This study aims to analyse the dynamics of the air-breathing PEMFC under Riyadh's monthly ambient conditions with respect to the overall performance, and the temperature and water distribution inside the stack. In additional to that, the effect of anode humidification on the performance of the PEMFC is examined. The work has been made in an attempt to help policy makers to consider implementing this technology in the public transport project.

Generally, the ambient conditions in Riyadh are sweltering and arid in the summer period, and cool and dry during winter. The temperature and humidity data used in this study were of year 2015. Throughout the year it's noted that the temperature ranges from as low as 9^{o}C in winter and to 43^{o}C in summer. Moreover the average relative humidity of air varies from 10% to 46% throughout the year. Graph 1 shows the profile data of the ambient conditions in Riyadh.

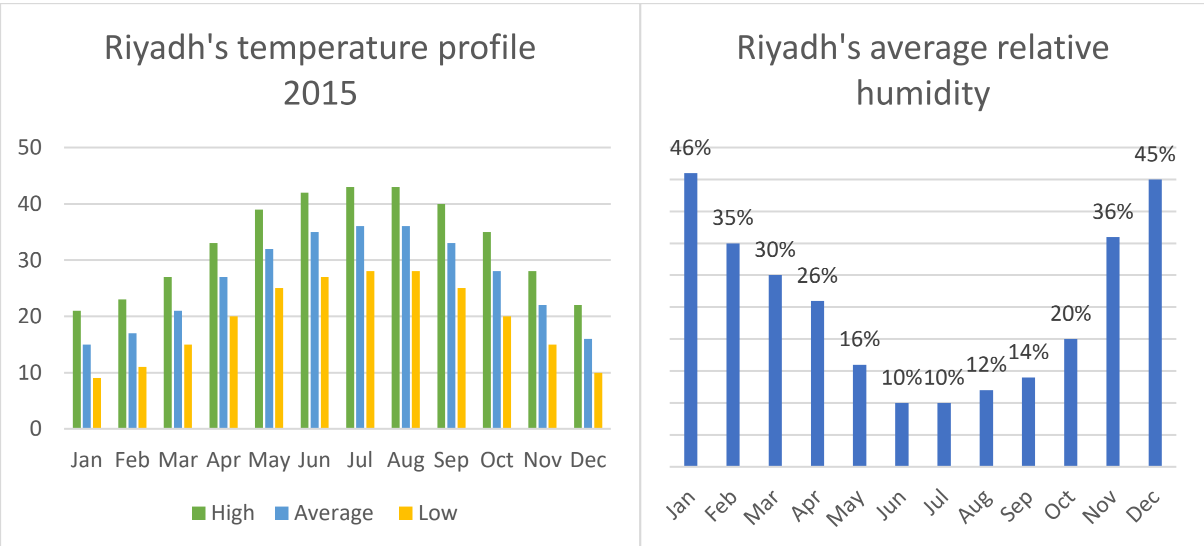


Figure 6. Monthly ambient data for Riyadh's city

MODEL DEVELOPMENT

In this study, one channel of PEMFC stack and ambient conditions is considered. The physical model of the PEMFC consist of two channels, also acting as current collectors, two diffusion layers, two catalyst layers and a thin membrane as illustrated in figure 7. The total dimensions of the model are 2.4 × 2.88 × 125 mm. Table 1 shows the dimensions of the elements in the model.

Table 1. Geometry data of the PEMFC's components model

Component	Dimensions (mm)
Channel	0.1 × 0.1 × 0.1
Diffusion layer	2.4 × 0.21 × 125
Catalyst layer	2.4 × 0.012 × 125
Membrane	2.4 × 0.036 × 125

The anode and cathode channels were run in a counter-flow mode, and the temperature of the boundaries were assumed to be constant in both directions. The model takes account of the following transport phenomena:

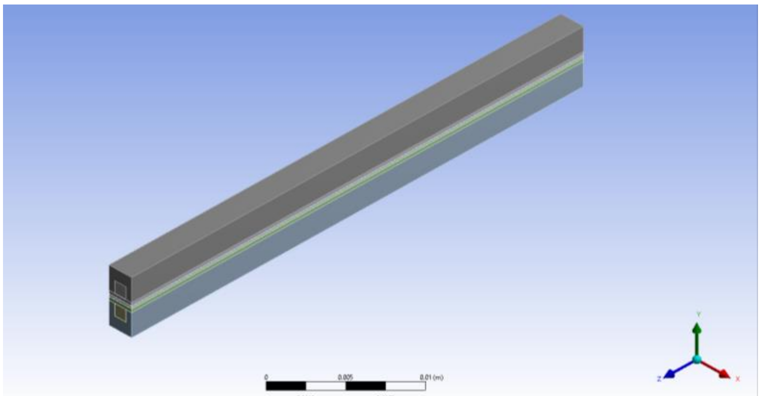


Figure 7. PEMFC model

1- Conservation of mass, momentum and species transfer of the two-phase is considered. The liquid in the model is assumed to be only water
2- Electrochemical reaction at the catalyst layer based on Bulter-Volmer expression.
3- Conservation of electrons and proton transport, and considering Ohm’s law.
4- Heat convection and conduction are considered in the model. Additionally, vaporisation, condensation, and entropy generation as a result of the chemical reaction are considered.
5- Water transport in the membrane is taking into account. Electro-osmatic drag, diffusion and absorption of water molecules are considered. Furthermore, Capillary action of liquid water is considered to dominate in the gas diffusion and catalyst layers.

Governing equations

The mathematical model used solves for conservations expressions of mass, momentum, energy, of the species (H_2, O_2, and H_2O) in two-phase states of the PEMFC with the surroundings. The model also includes three additional conservations equations for multiphase flow, electrochemistry and current transport. The membrane in the model is the crucial part and has two main roles: transporting oxygen ions from the cathode to the anode, and blocking gas flow and electrons from flowing through the two terminals. The flow of electrons in an external circuit (electronic charge) balances with the ions that are flowing through the membrane, when a load is connected and an electrical power is being produced [18]. The main governing equations are summarised as follows:

$$\nabla \cdot (\rho^g u^g) = S_{mass} - \dot{m_{H_2O}} \tag{1}$$

Equation 1 represent the mass conservation for the gases and the liquid water inside the fuel cell, where ρ^g denote the phase density of the mixture gasses, u^g is the 3 dimensional velocity vectors of the mixture, and m_{H_2O} is the interphase mass transfer of H_2O between the two phases. The source term S_{mass} represent the consumption/production rate of the electrochemical reaction of gases at the catalyst layer. In the PEMFC model, it corresponds to H_2 consumption and H_2O production at the anode active layer, and O_2 consumption at the cathode active layer. Each source term is expressed as follows:

$$S_{mass-anode} = \left(J_{H_2} + J_{H_2O}\right) \cdot \frac{A_{active}}{V} = \left(-\frac{I_{Anode}}{2F} M_{H_2} + \frac{I_{Anode}}{2F} M_{H_2O}\right) \frac{A_{active}}{V} \tag{2}$$

$$S_{mass-cathode} = J_{O_2} \cdot \frac{A_{active}}{V} = -\frac{I_{Cathode}}{4F} M_{O_2} \cdot \frac{A_{active}}{V} \tag{3}$$

For the momentum transport conservation, Navier-Stokes equations are used to express fluid flow through channels, and Darcy's term is added to solve porous electrodes [19]. The former equation is applied as it describes the physics of laminar and turbulent incompressible flow well, and such assumption is made due to the low velocities of the inlet reactants. The expression for momentum is therefore;

$$\nabla(\rho^g U^g U^g) = -\nabla P + \nabla(\mu^g \nabla U) + S_d \tag{4}$$

Where P and μ^g are the pressure and viscosity of the mixture gasses respectively.

The heat conservation equation is expressed as follows:

$$\nabla \left(\rho^g C_p^g u^g T\right) = \nabla \cdot \left(k_{eff} \nabla T\right) + S_T \tag{5}$$

Where k_{eff} and C_p^g are the effective thermal conductivity and effective specific heat of the mixture gasses respectively. This equation balances heat conduction between the solid zone and reactants, convective energy, heat flux due to reactants diffusion and the source term.

Poisson's equations are applied to express the charge conservation expression for electronic and ionic phase:

$$-\nabla\left(\sigma_{eff} \nabla \emptyset\right) = S_{\emptyset} \tag{6}$$

Where σ_{eff} is the effective electronic/ionic conductivity in the membrane, and $S_{\emptyset}$ is the source term of the transfer current between the ionic and electronic phases at the active layers.

The open circuit voltage for the electrochemical reaction is determined using Nernst equation, expressed as follows:

$$Voltage_{open-circuit} = E^{\circ} - \frac{RT}{2F} \ln\left(\frac{P_{H_2O}}{P_{H_2}\sqrt{P_{O_2}}}\right) \tag{7}$$

Where E° denotes the potential at the standard temperature and pressure, $P_{component}$ is the partial pressure for every component in the system, R is gas constant, T is the operating temperature of the fuel cell, and F is the Faraday's constant.

Boundary conditions

The boundary conditions in the model were set as follows:

- At the cathode terminal, we set the operating cell voltage of the PEMFC stack, and temperature to be fixed to surrounding conditions.

$$\emptyset^{s} = E_{operating} \quad T_{sur} = T_{Cathod-inlet} \tag{8}$$

- At the anode terminal, we have set the voltage to be zero, and temperature was fixed to surrounding conditions.

$$\emptyset^{s} = 0 \quad T_{sur} = T_{Anode-inlet} \tag{9}$$

- At the cathode inlet zone, the ambient conditions were for the species were assumed. The water content of air was obtained from the relative humidity at a specific condition and was set.

$$P^{g} = P_{amb}\ \omega_{O_2} = \omega_{O_2}^{amb}\ \omega_{H_2O} = \omega_{H_2O}^{amb}\ T = T_{amb} \tag{10}$$

- At the cathode outlet zone, fluxes of the species, temperature and liquid fraction were set to zero at the direction vector of 1 in the z-axis.
- At the anode inlet, the mass flow rate of hydrogen was set in the stiochmetric ratio 1:2, and the temperature was fixed to the ambient conditions.
- At the anode outlet zone, fluxes of the species, temperature and liquid fraction were set to zero at the direction vector of -1 in the z-axis.

NUMERICS AND PARAMETERS

The computational model (as shown in figure 6) was created, and then meshed in the the pre-processor software tool Ansys ICEM 17.1, with around 3×10^{6} elements. The mathematical formulation is then solved in a one-domain approach using the commercial CFD tool Ansys Fluent 17.1 and its add-on PEMFC module. The number of iterations for each set is 1,800 with a convergence criteria of 0.0001 for all residuals. The simulation parameters used were based on the study conducted by Iranzo [20] which was verified experimentally and proved to show good prediction of the PEMFC behaviour. Table 2 shows the list of the parameters. Furthermore, all the options in the PEMFC module were selected except for anisotrpic conductivity and multicomponent diffusion to decrease complexity of calculation.

Table 2. Used simulation parameters

Parameter	Value	Parameter	Value	Parameter	Value
BP density	1990 kg/m^3	GDL electric conductivity	280 1/(Ω·m)	Membrane equivalent weight	1100 kg/kmol
BP specific heat capacity	710 J/(kg·K)	GDL viscous resistance (anode)	1.00 x10^{12} 1/m^2	Open circuit voltage	0.95 V
BP thermal conductivity	120 W/(m·K)	GDL viscous	3.86 x10^{12}	H_2 diffusivity	8.0x10^{-5}

		resistance (cathode)	$1/m^2$		
BP electric conductivity	92,600 $1/(\Omega\cdot m)$	GDL wall contact angle	110 deg	O_2 diffusivity	2.0 $x10^{-5}$ m^2/s
BP GDL contact resistance	4.56 $x10^{-6}$ $\Omega\cdot m^2$	CL surface-to-volume ratio	1.25 $x10^7$	H_2O diffusivity	5 .0$x10^{-5}$ m^2/s
GDL density	321.5 kg/m^3	Membrane density	1980	Pore blockage saturation exponent	2
GDL porosity	0.82	Membrane thermal conductivity	0.16	Concentration exponent (anode)	0.5
Reference exchange current density (anode)	$4.48x10^5$ A/m^2	Reference exchange current density (cathode)	4.48 A/m^2	Concentration exponent (cathode)	1

RESULTS & DSCUSSION

Computational fluid dynamic simulation was carried out to analyse the performance of air-breathing PEMFC stack subject to typical Riyadh's ambient conditions. The model was simulated under three main sets of ambient conditions, which are listed in table 4. For the first study the anode inlet was assumed to be dry and pure hydrogen to see the effect of ambient conditions solely on the operation of the PEMFC. The second study involves the evaluation of anode humidification.

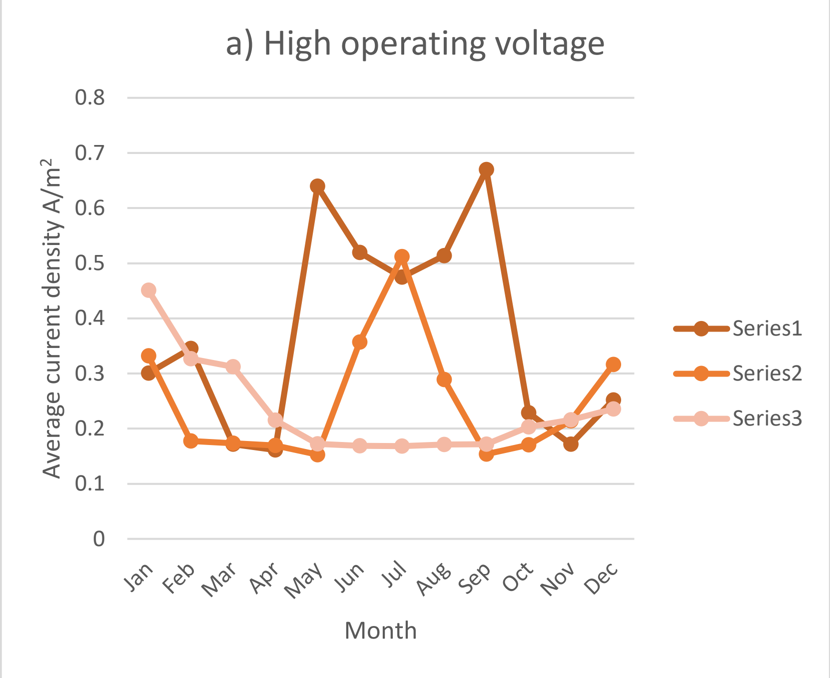
Table 3. Combinations of sets used in the simulation

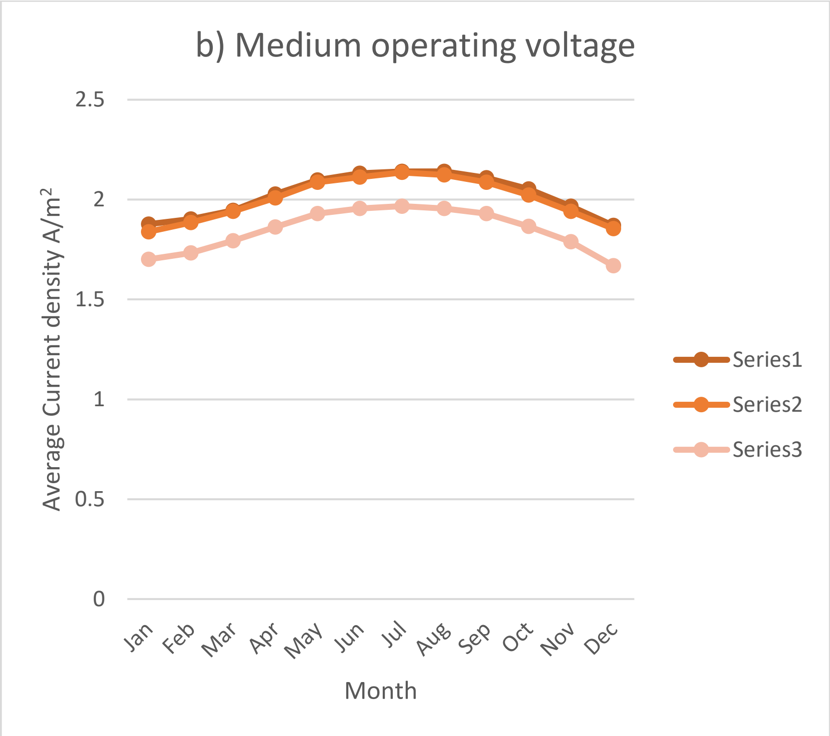
	Temperature	Relative humidity
Set 1	High	Average
Set 2	Average	Average
Set 3	Low	Average

Effect of ambient conditions

For each set, three different operating voltages were considered to mimic the dynamics of vehicles due to acceleration and deceleration. The loads were assumed to be constant for simplicity. The considered voltage values are: high 0.75 V, medium 0.55 V, and low 0.35 V. The high voltage represent the deceleration stage where current is drawn at low amounts. Oppositely, low voltage represent the acceleration stage where high current is generated in the stack. The medium voltage is where the optimum efficiency of the PEMFC is typically found, and thus is the desired option for steady speeds.

Figure 3 demonstrates the monthly-generated current densities for the three combinations of sets at the three operating voltages. It has noted that at the high operating voltage and high load, the trends for the three sets does not follow the same pattern. This is attributed to the lower temperature rise of the stack (less current is being drawn), which reduces the reaction kinetics of the PEMFC making it insufficient to overcome the ionic resistance of the membrane. It can be clearly seen that set 3 (lowest temperature) has a greater performance than set 1 (highest temperature) from January to April, this is due to the more water content of the membrane which decreases the ionic resistance. The performance for set 1 at high voltage, considerably increase in May, and this is where the summer begins and the temperature becomes high enough for the reaction kinetics to outcome the overall ohmic resistance. Overall, the performance of the PEMFC under Riyadh's ambient conditions is best during the summer time (May-Sep) as it can be clearly seen from figure 8. The performance has been observed to be improved by around 28% from cold humid conditions in December to hot and dry conditions in July.





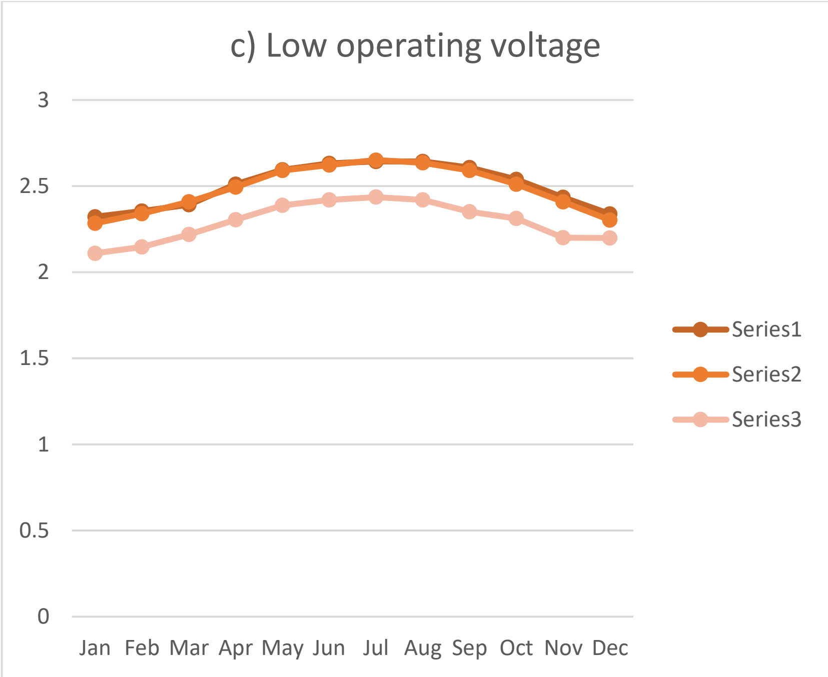
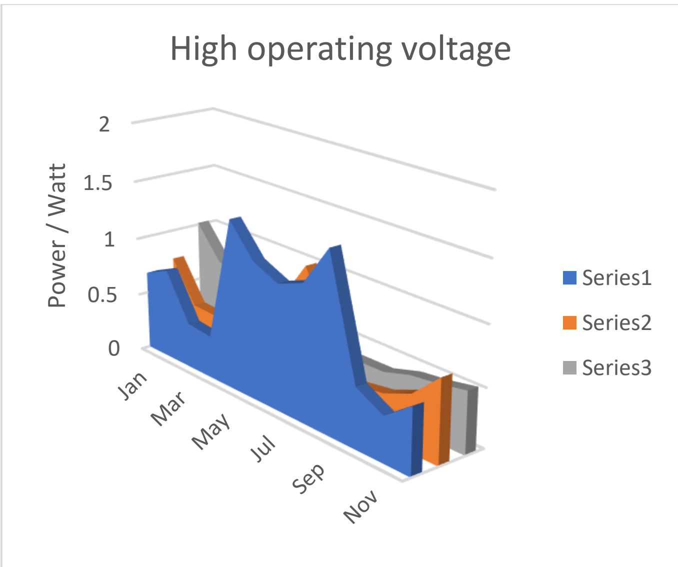


Figure 8. Current densities for a PEMFC operates at a) High b) Medium c) Low voltages

In addition, Figure 9 was plotted to the output power generated by the stack at the three combinations of sets under the three operating voltages and the values were obtained by using the following equation:

$$P_{stack} = V_{operating} \cdot J \cdot A_{ative} \tag{11}$$

It can be noted that overall, set 1 (high temperature) generate the best performance. At high operating voltage, the output power of the stack varies between 0.35W to 1.5 W, this indicate that the performance of the PEMFC, is strongly influenced by the ambient conditions. At the medium voltage, the highest output power is achieved, and it is observed to be ranging from 2.75W to 3.50W in our model.



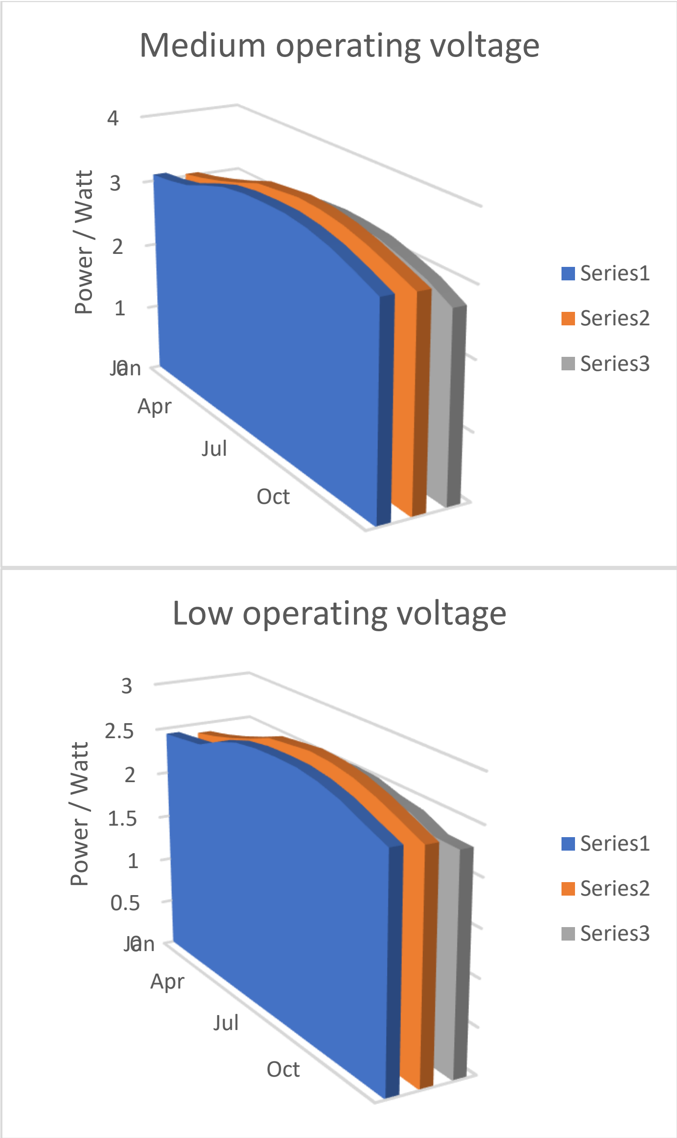


Figure 9. Power output of the PEMFC operating at a) High b) Medium c) Low voltages

Effect of Anode humidification

Water content per sulfonic group of the membrane plays a crucial role in minimising resistance losses across the membrane. Humidifying hydrogen is applied to maintain good water management as drying of membrane is often occur in the anode side, due to the electroosmotic drag.

In this section, the effect of 100% humidification of hydrogen on the performance of PEMFC stack is evaluated under extremely dry and hot conditions (July month). Figure 10 shows the polarisation curve for both cases. As it can be seen the humidified anode gives a better fuel cell performance and this is due to the increased hydration of the membrane which result in a better protonic conductivity. It's also noted that the effect of anode humidification becomes more significant when operating at a lower voltage.

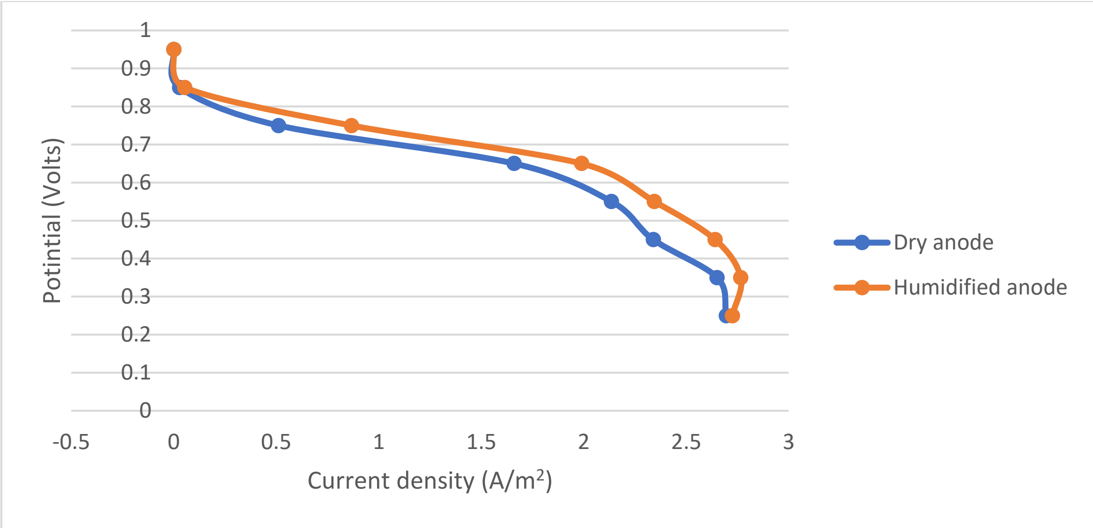


Figure 10. Polarization curves for humid and dry conditions.

Additionally, the water content profiles, in the cathode side of membrane, for both cases are illustrated in figure 11. As it can be clearly seen, the water profile is denser for the humidified case, which confirms that membrane is more hydrated.

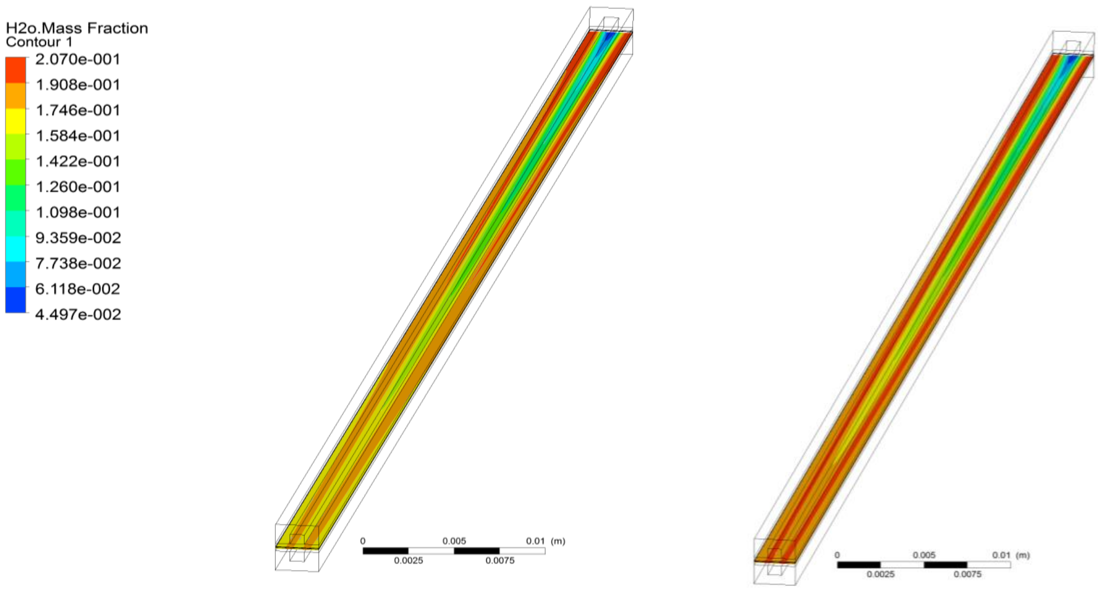


Figure 11. Water content of membrane in cathode side of the PEMFC for anode and humidified conditions.

CONCLUSUON

In conclusion, this paper presented the results of finite element method computational analysis on the effect of ambient conditions of Riyadh on the performance of an air breathing PEMFC. Also anode humidification was examined to see the impact of the performance on the PEMFC stack and water management. It was noted that ambient conditions, i.e. temperature and humidity of air plays a vital role in the output power of the stack. The results showed that the power is increased by 28% during hot and arid conditions as opposed to cold conditions.

Furthermore the heat generated in the stack, especially at low currents, was observed to maintain fast reaction kinetics and overcoming the membrane resistance.

This work is limited to a single channel at a steady state model using monthly ambient data. Future work will involve simulation of a full stack at a dynamic loadings, which are typically found in driving scenarios.

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